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Spherical Target Temperature by Extended CFAST Calculation

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1. Introduction

The purpose of this calculation is to evaluate the temperature at the surface of a spherical target made of polyethylene during a room fire.

The current calculation is separated into 2 steps:

- CFAST code calculation:
  Calculate the air temperature; radiation flux to the target from the fire, surrounding air, and walls; convection flux; and target temperature.

- Extended model calculation:
  Calculate the temperature of the target sphere taking into account the density, heat capacity, heat conductivity, and the spherical geometry of the target by solving the coupled finite difference equations. The second step calculation utilizes the air temperature and radiation flux determined by the CFAST code calculation in the first step.

2. CFAST Code Calculation

The CFAST code (Version 6.0.10) is used to perform the fire analysis [1, 2].

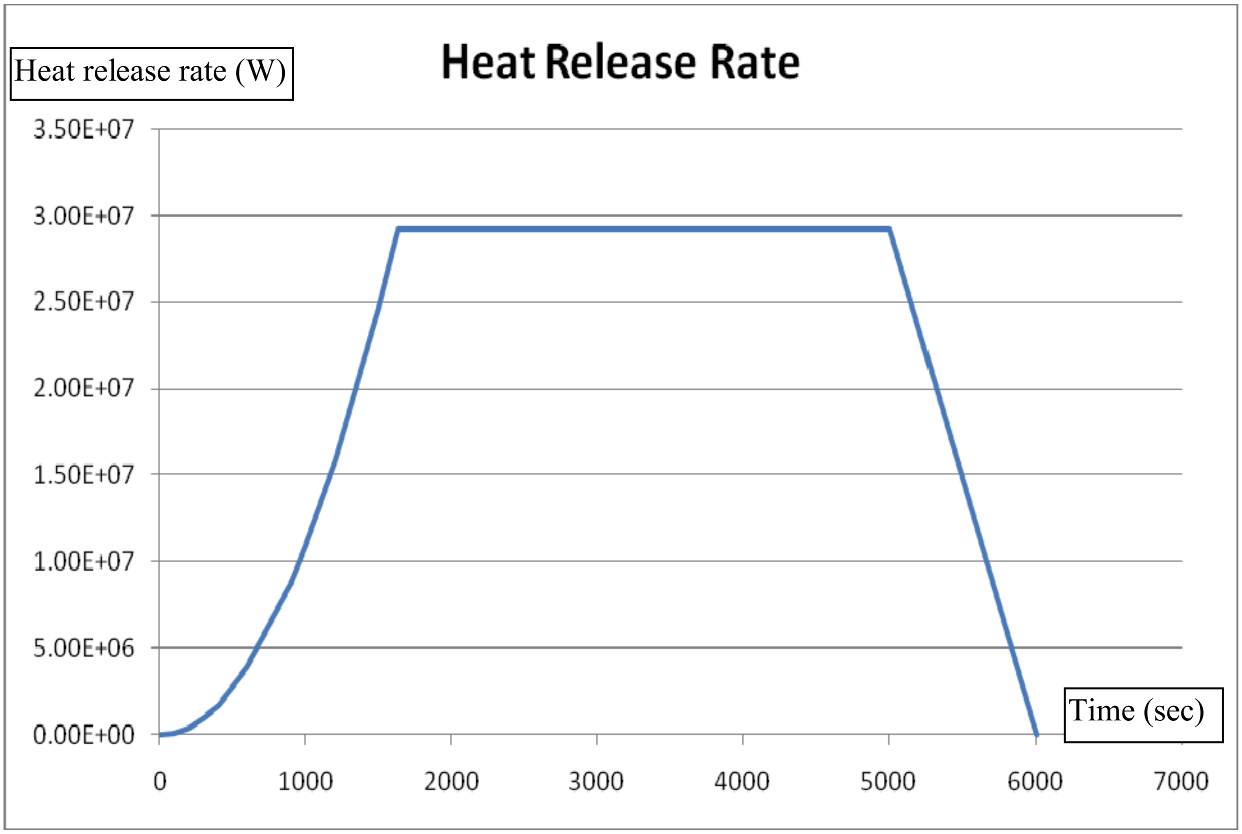
Inputs

The following are the major inputs used in the calculation:

- The dimension of the Room is 50 x 50 x 30 ft.
- The ventilation rate is 400 cfm , there are no other openings (door, window) to outside.

- The target sphere is placed at the room center and sitting on a 1 ft stool. The diameter of the sphere is 1 ft. A fire is assumed to occur at 8 ft from the target sphere.
- The fire is taken to be a medium growth fire, t_g = 310 sec. The heat release rate is depicted in Figure 1.

Figure 1 Heat release rates, Q, under free ventilation condition.



Result

The CFAST code is able to calculate the temperature of a target during a fire using various options. The results of maximal temperatures at time = 1020 sec are shown below:

Calculated peak temperature of the target by CFAST code.

Type / Method	Thin	Thick
Steady	542 °C	542 °C
Explicit	606 °C	-infinity
Implicit	605 °C	536 °C

Upper zone max. temp. = 365 °C, at 1020 sec.

The calculated maximal temperatures of the target using various options are all larger than 350 °C, which is the self ignition temperature of polyethylene. This implies that the target sphere of polyethylene will self ignite due to a fire 8 ft away.

It should be emphasized that in the CFAST code steady state calculation, the temperature at the surface of the target is determined solely by the energy balance of the radiation and the convection at the target surface. In reality, however, the target is a heat sink with a non-zero density, heat capacity, and heat conductivity. As a result, the steady state target temperature determined by the CFAST code is very conservative.

The following section takes into account the heat capacity, heat conduction, density, and the spherical geometry of the target in addition to the radiation, air convection, and melting; thus yielding a more realistic temperature of the target.

3. Extended Model Calculation

The CFAST code is able to calculate the temperature of a target during a fire in a steady state based on the energy balance of the radiation and convection at the target surface, i.e.:

outgoing energy at the target surface = incoming energy at the target surface

This energy balance yields:

$$\Delta A \cdot \varepsilon \, \sigma \, T^4 = \Delta A \cdot Q_{\text{radiation absorption}} + \Delta A \cdot Q_{\text{convection}} \qquad (1)$$

where $\varepsilon = 0.9$ is the emission coefficient for target materials, $\sigma = 5.67 \times 10^{-8}$ W/m^2-K^4 is the Stefan constant, T is the temperature (in K) at the target surface, ΔA is the surface element.

$$Q_{\text{radiation absorption}} = \alpha \, (\text{fire radiation flux} + \text{wall radiation flux} + \text{gas radiation flux}) \qquad (2)$$

where $\alpha = 0.9$ is the absorption coefficient for the target materials.

$$Q_{\text{convection}} = h\,(T_{\text{convc}} - T) \qquad (3)$$

where h is the convective coefficient. which is a complicated function that depends on system, fluid medium, temperature, etc. T_{convc} is the temperatures of the convective air surrounding the target.

The heat conduction equation for the spherical target without a heat source is:

$$\rho C_p \frac{\partial T}{\partial t} = k \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) \qquad (4)$$

heat conduction inside the sphere

temp. change of the sphere

where ρ, C_p, and k denote the density, heat capacity, and heat conduction coefficient of the sphere, respectively.

Differentiating the right hand side gives:

$$\rho C_p \frac{\partial T}{\partial t} = k \frac{2}{r}\frac{\partial T}{\partial r} + k \frac{\partial^2 T}{\partial r^2} \tag{5}$$

This partial differential equation can be translated into a set of coupled finite difference equations [3].

Consider first the finite difference approximation in the space dimension by dividing the sphere into N equal radial intervals:

$$\Delta r = \frac{R}{N}, \qquad r_m = m\,\Delta r, \qquad m = 1,2,\ldots..,N$$

where R is the radius of the sphere.

Define:

$$\frac{\partial T_m}{\partial r} \cong \frac{T_{m+1} - T_{m-1}}{2\Delta r},$$

$$\frac{\partial^2 T_m}{\partial r^2} \cong \frac{1}{\Delta r}\left(\frac{T_{m+1} - T_m}{(\Delta r)} - \frac{T_m - T_{m-1}}{(\Delta r)}\right) = \frac{T_{m+1} - 2T_m + T_{m-1}}{(\Delta r)^2}$$

The differential equation (4) becomes:

$$\rho C_p \frac{\partial T_m}{\partial t} = \frac{k}{(\Delta r)^2}\left[(1+\frac{1}{m})T_{m+1} - 2T_m + (1-\frac{1}{m})T_{m-1}\right] \tag{6}$$

Note that Eq. (6) applies only to the interior region of the sphere. Let's take N=10; thus Eq. (6) applies only to m = 1, 2, ……..9. For the surface layer (i.e., m=10), one obtains:

$$\underbrace{\Delta V \cdot \rho C_p \frac{\partial T_{10}}{\partial t}}_{\text{temp. change of the volume element } \Delta V \text{ in the surface layer}} = \underbrace{\Delta A \cdot \frac{k}{\Delta r}(T_9 - T_{10})}_{\text{heat conduction from the surface layer to the interior region}} + \underbrace{\Delta A \cdot Q_{radiation\ \mathrm{absorption}}}_{\text{radiation absorption from fire, surrounding gas, and walls by the surface layer}} + \underbrace{\Delta A \cdot Q_{convection}}_{\text{convection between the surface layer and the surrounding gas}} - \underbrace{\Delta A \cdot \varepsilon\sigma\, T_{10}^{\ 4}}_{\text{radiation emission from the surface layer to the surroundings}} \tag{7}$$

where $\Delta V = \Delta A \cdot \Delta r$.

Note that if one assumes $C_p = 0$ and $k = 0$; Eq.(7) reduces to Eq.(1).

Next, applying the finite difference approximation to the time dimension, one obtains:

$$\Delta T_m(t_i) = T_m(t_{i+1}) - T_m(t_i)$$

$$\Delta t = t_{i+1} - t_i$$

For m = 1 to 9, Equation (6) becomes:

$$T_m(t_{i+1}) = (1 - \frac{2k\Delta t}{\rho C_p (\Delta r)^2}) T_m(t_i) + \frac{k\Delta t}{\rho C_p (\Delta r)^2}\left[(1+\frac{1}{m})T_{m+1}(t_i) + (1-\frac{1}{m})T_{m-1}(t_i)\right] \qquad (8)$$

For m = 10, Equation (7) becomes:

$$\begin{aligned} T_{10}(t_{i+1}) &= T_{10}(t_i) + \frac{k\Delta t}{\rho C_p (\Delta r)^2}[(T_9(t_i) - T_{10}(t_i)] \\ &+ \frac{\Delta t}{\rho C_p \Delta r}[Q_{radiation\ \mathrm{absorption}}(t_i) + Q_{convection}(t_i) - \varepsilon\sigma T_{10}(t_i)^4] \end{aligned} \qquad (9)$$

The initial condition is:

$T_1 = T_2 = \ldots\ldots\ldots = T_9 = T_{10} = 20$ °C.

The parameters used to perform the extended CFAST model are listed in Table 1.

Table 1 Parameters for polyethylene.

Density ρ (g/m3)	9.50E5[1]
Specific heat capacity C_p (J/g-°C)	2.3[2]
Conductivity k (W/m-°C)	0.4[2]
Self ignition temperature (°C)	349[2]
Melting temperature (°C)	120 - 140[2]
Fusion energy H_f(J/g)	286[3]
Molecular weight (g/mol)	28.05[3]
Emisivity ε	0.9[6]
Stefan const σ (W/m^2-K^4)	5.67E-8

Sources:

1. Program information; see also J. Brandrup, E.H. Immergut, and E.A. Grulke, “Polymer Handbook”, 4th Edition, 1999. Page VI/8.
2. A. H. Landrock, “Handbook of Plastics Flammability and Combustion Toxicology”, 1983. C. Hilado, “Flammability Handbook for Plastics”, 1969.

3. J. Brandrup, E.H. Immergut, and E.A. Grulke, "Polymer Handbook", 4th Edition, 1999. Page VI/8.
   Polyethylene: H_f = 8.03 kJ/mol = 8.03 kJ/28.05 g = 286 J/g
4. J. Brandrup, E.H. Immergut, and E.A. Grulke, "Polymer Handbook", 4th Edition, 1999. Page V/87.
5. J. Brandrup, E.H. Immergut, and E.A. Grulke, "Polymer Handbook", 4th Edition, 1999. Page V/167. It is stated that the 105°C as quoted in Landrock (Table A.8, Ref. 2) is the glass transition temperature not the melting temperature.
6. Emisivity of urethane is used, CFAST data base: thermal.csv

Radiation flux

The radiation absorption flux, $Q_{radiation\ absorption}$ (see Eq.2) depends solely on the temperatures of the fire, walls, and the surrounding gas, and does not depend on the temperature of the target sphere. Thus the radiation flux calculated by the CFAST code can be readily used in the current calculation.

Convection flux

The convection flux, $Q_{convection}$ (see Eq.3), depends on the temperatures of the convective air surrounding the target, T_{convc}, and the temperature of the target surface T_{10}.

The convection flux (together with the radiation flux) is calculated by the CFAST code; however, the CFAST code calculated convection flux can't be used in the current calculation. This is because the temperature of the target calculated by the CFAST code is different from that of the target surface, T_{10}, under consideration here, although the air temperature calculated by the CFAST code is still valid.

Following the approach of the Fire Protection Engineering Handbook [4], the convection flux for a sphere is recalculated for a few typical temperatures that are within the range of interest of the current calculation; the results are listed in Table 2. Table 2 shows that the value of the convective coefficient, h, ranges from 5.2 to 7.3 W/m^2-K in the range of interest. In order to avoid a full calculation of heat convection which is less than 10% of the radiation term (see Table 2), a conservative value of 8 W/m^2-K is assumed in this calculation.

Melting

When a volume element ΔV of the target surface reaches the melting temperature, T_{melt}; the temperature will stay constant at T_{melt} until the element is totally melted by supplying the fusion heat $\rho \cdot \Delta V \cdot H_f$ to the volume element. During melting, the total absorption heat must equal the fusion heat before the temperature can raise again; i.e.:

$$\Delta A\{\frac{k}{\Delta r}[(T_9(t_i) - T_{10}(t_i)] + Q_{radiation\ \ \text{absorption}}(t_i) + Q_{convection}(t_i) - \varepsilon\sigma\, T_{10}(t_i)^4\}\Delta t = \rho\, \Delta V H_f \qquad (10)$$

Table 2 Air convection flux.

						Sphere		
T-convc	T-10	ν	k	α	Ra-D	Nu	h	Convc flux
(°C)	(°C)	(1E-6 m2/sec)	(1E-3 W/m-K)	(1E-6 m2/s)			(W/m2-K)	(W/m2)
100	50	2.07E+01	2.99E+01	2.96E+01	6.50E+07	4.69E+01	4.59E+00	2.30E+02
150	50	2.34E+01	3.17E+01	3.38E+01	9.40E+07	5.12E+01	5.34E+00	5.34E+02
200	100	2.92E+01	3.54E+01	4.24E+01	5.31E+07	4.47E+01	5.19E+00	5.19E+02
300	100	3.53E+01	3.89E+01	5.16E+01	6.44E+07	4.68E+01	5.97E+00	1.19E+03
400	100	4.19E+01	4.22E+01	6.13E+01	6.20E+07	4.64E+01	6.41E+00	1.92E+03
300	150	3.85E+01	4.06E+01	5.63E+01	3.85E+07	4.14E+01	5.51E+00	8.26E+02
400	150	4.53E+01	4.38E+01	6.63E+01	4.22E+07	4.23E+01	6.07E+00	1.52E+03

Result

An EXEL spread sheet is developed to perform the extended model calculation (see Eqs. 8, 9, and 10). The results are listed below:

Calculated peak temperature at the target surface.

CFAST code (Steady State)	Extended Model
542 °C (at 1020 sec)	143 °C (at 1110 sec)

4. Conclusion

The peak temperature at the surface of a target sphere during a room fire is calculated by the CFAST code as well as by an extended model. The results of the CFAST code is very conservative; while the extended model takes into account the heat capacity, heat conduction, density, and the spherical geometry of the target as well as the radiation, convection, and melting; thus yielding a lower and more realistic peak target temperature. This calculation indicates that care must be taken in interpreting the target temperature calculated by the CFAST code.

5. References

1. R. D. Peacock, W. W. Jones, P. A. Reneke, and G. P. Forney, CFAST – Consolidated Model of Fire Growth and Smoke Transport (Version 6), User's Guide, NIST Special Publication 1041, U.S. Department of Commerce, 2005.
2. W. W. Jones, R. D. Peacock, G. P. Forney, and P. A. Reneke, CFAST – Consolidated Model of Fire Growth and Smoke Transport (Version 6), Technical Reference Guide, NIST Special Publication 1026, U.S. Department of Commerce, 2005.
3. N. Necati Ozisik, Finite Difference Methods in Heat Transfer, CRC Press, 1994.
4. A. Atreya, "Convection Heat Transfer", Chapter 3 in the SFPE Handbook of Fire Protection, 3rd ed, SFPA,2002.